

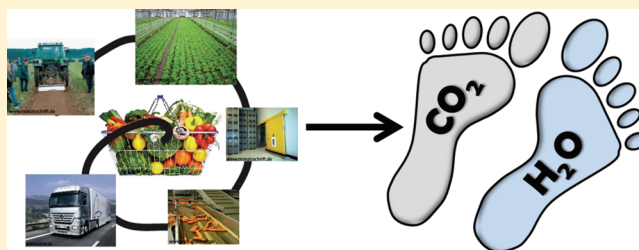
Life Cycle Inventory and Carbon and Water FoodPrint of Fruits and Vegetables: Application to a Swiss Retailer

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S Supporting Information

ABSTRACT: Food production and consumption is known to have significant environmental impacts. In the present work, the life cycle assessment methodology is used for the environmental assessment of an assortment of 34 fruits and vegetables of a large Swiss retailer, with the aim of providing environmental decision-support to the retailer and establishing life cycle inventories (LCI) also applicable to other case studies. The LCI includes, among others, seedling production, farm machinery use, fuels for the heating of greenhouses, irrigation, fertilizers, pesticides, storage and transport to and within Switzerland. The results show that the largest reduction of environmental impacts can be achieved by consuming seasonal fruits and vegetables, followed by reduction of transport by airplane. Sourcing fruits and vegetables locally is only a good strategy to reduce the carbon footprint if no greenhouse heating with fossil fuels is involved. The impact of water consumption depends on the location of agricultural production. For some crops a trade-off between the carbon footprint and the induced water stress is observed. The results were used by the retailer to support the purchasing decisions and improve the supply chain management.



INTRODUCTION

Recent studies have shown that food production and consumption are responsible for 10–30% of an individual's total environmental impact.^{1–3} A considerable amount of the total food intake by mass (30%) is represented by fruits and vegetables, which constitute the largest food group consumed worldwide.⁴ The effects of their production are revealed in different categories of environmental impacts, like climate change, impacts of land and water use, human- and eco-toxicological effects, eutrophication, acidification, soil fertility degradation, and landscape changes. Policy makers and private companies in various countries have recognized the need to quantify these environmental impacts and, on this basis, to identify measures for impact reduction. For instance, a new law in France⁵ and a recommendation of the Swiss Federal Office for the Environment⁶ encourage the labeling of food products with their carbon/environmental footprints. Private companies, such as Tesco and Walmart, calculate the carbon footprint of some of their products and communicate these to their customers,⁷ while others use such environmental information for internal decision making regarding products and supply chain management.⁸ Finally, water footprint studies have gained high interest in the area of food production,^{9,10} revealing the amounts of water consumption and the related impacts. The International Organization for Standardization (ISO) is therefore currently considering a standard on water footprint to allow consistent analysis and reporting for product labeling.¹¹ Despite these initiatives there are still large data gaps concerning the environmental assessment of food products. For instance, while several life cycle assessment (LCA) studies on a variety of fruits and

vegetables have been published,^{12–17} the comparability of these studies is compromised by differences in system boundaries and background data. In contrast to process-based LCA studies, input-output LCA studies^{18,19} provide data on total food consumption without having cut-offs in the supply chain, leading to a large gap in the overall impacts. Such studies help to identify relevant food groups, but the data are given on an industrial-sector resolution and hence do not allow for identifying improvement potentials within sectors. Moreover, international trade is not well captured due to inconsistencies in the underlying statistical data. Thus, in addition to these studies, detailed, process-based LCA data are needed to support decisions regarding adequate sourcing of food products, means of transportation, agricultural management, and, finally, choices between different food commodities. The goals of the present study were (a) to elaborate a consistent and up-to-date life cycle inventory (LCI) of a large range of fruits and vegetables from different origins, (b) to show selected life cycle impact assessment (LCIA) results and derive general decision guidelines for producers, retailers, policy makers and consumers on how to improve the environmental impacts of fruit and vegetable consumption, and (c) to illustrate and discuss the implementation of these guidelines for a specific case of purchasing decision and environmental supply chain management of a main Swiss retailer.

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MATERIALS AND METHODS

System Boundaries. The functional unit (FU) was defined as 1 kg of product at the point of sale. The LCA study includes the following fruits and vegetables: apple, avocado, banana, broccoli, cabbage for preserves, carrots, cauliflower, celery root, citrus fruits, cucumbers, eggplant, fennel, grape, green asparagus, bell pepper, iceberg lettuce, kiwi, lettuce, melon, onion, vine tomatoes, papaya, pear, pineapple, potatoes (LCI adapted from ecoinvent²⁰), radish, red cabbage, round carrots, spinach, strawberries, tomatoes, white asparagus, white cabbage, and zucchini. These products cover more than 80% of the fruits and vegetables sold by one of the two major retailers in Switzerland in 2007, for which the study was originally undertaken. The products were either produced locally or transported to Switzerland from 29 different countries. The LCI were compiled by extrapolating from a basic set of data for one product to the same product from other origins by varying parameters, such as transport means and distances, irrigation, heating energy for greenhouse production, and cooling energy for storage. Inputs and outputs from packaging and the operation of the store were excluded from the analysis as these were shown to be relatively low compared to the overall impact (Supporting Information (SI), section 1) and equal for all fruits and vegetables. Vegetables, apples, pears and strawberries were modeled using the Swiss agricultural standard production scheme called “integrated production” as described elsewhere.²¹ The other fruits were produced according to the so-called “conventional production”. The system boundaries are shown in Figure 1.

Data Sources and Assumptions for LCI Analysis. Tables with agricultural production means for cost calculations were used to set up the inventory of vegetables,²² apples and

pears,²³ whereas for tropical fruit production additional data were obtained from literature and leaflets of agricultural extension services (SI, section 2). Good agricultural practice (GAP) was assumed for all agricultural activities, irrespective of the production site, assuming common global standards throughout the supply chain. This assumption was in accordance with the commissioner of the study, but may need to be revised in cases in which retailers do not make sure that GAP is applied. Modeling was done with SimaPro 7 using background processes from ecoinvent v. 2.01.²⁰ Next, a short outline of every parameter considered in the LCI is given; detailed information can be found in the SI, section 2.

Yields/Land Use. It was assumed that the land occupied is arable and that it had been used for agriculture for a long time. Therefore no impacts caused by land transformation were taken into account. Land occupation was calculated based on yield and cultivation time per kg of product (SI, section 3).

Vegetable Seedlings. One of the upstream processes of vegetable growing is the production of seedlings, which are young plants to be bedded out. They are grown in pots, mainly filled with peat. In this study we assumed an average size of 20 cm³ per pot²⁴ with an estimated weight of 20 g. Based on the yield and number of seedlings planted per ha, the amount of peat and the transported weight per kg of product from the mining site were calculated.

Seedling production in Switzerland or further north is generally assumed to take place in heated greenhouses over five weeks. For heating oil consumption, the data for eggplants were assumed for all vegetable seedlings because of similar temperature requirements.

Fertilization. The nutrients, extracted by the plants, eroded and leached to water, have to be replaced by soil fertilization.

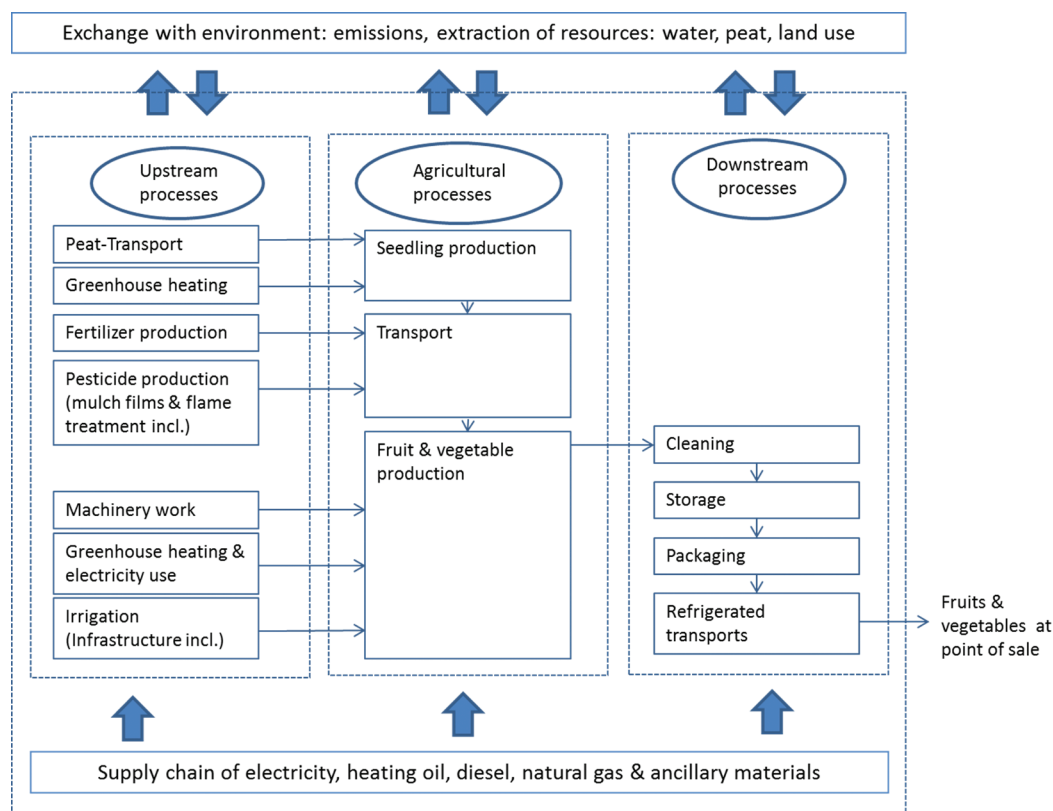


Figure 1. System boundaries for cradle-to-gate fruit and vegetable production.

Here we considered effective fertilization with macronutrients using the ecoinvent processes “ammonium nitrate”, “single super-phosphate as P_2O_5 ” and “potassium sulphate” (SI, section 5).

Pesticide Use. The use of 84 pesticide active ingredients was modeled. In most cases individual pesticide production data were not available. In such cases, the generic pesticide process “pesticide unspecified, at regional storehouse” from ecoinvent was used. Field emissions of pesticides are often farm-specific and models like in^{25,26} can be used to estimate such emissions accurately.

Farm Machinery Use. Farm machinery use facilitates field work. The ecoinvent data set “fertilizing by broadcaster” with middle intensive fuel consumption was used as a proxy for horticultural machinery. Data on the number of machinery operations and the working hours for running the machines were used to quantify the amount of machinery input per kg of crop (SI, section 8).

Electricity Use in Greenhouses. Greenhouse production implies electricity use, for example, for lighting and irrigation pumps. The electricity demand was estimated using information from Swiss cost calculation sheets²² assuming a price of 0.15 CHF/kWh for industrial companies. The average European electricity mix (ENTSO-E, former UCTE) of low voltage was used for all crops except those originating from the Americas, to which the U.S.-mix was applied.

Heating Oil Use in Greenhouses. Vegetables need to grow at specific temperatures. To be independent from outdoor temperature, greenhouses are built to provide the appropriate climate. To show the variability of fuel consumption related to seasonality, a time-dependent heating energy model for greenhouse production was developed and applied. This model considers the type of greenhouse (heat transmission properties), the building dimensions, the difference in outside and inside temperature required by the specific crop, solar irradiation and the yield. For details see the model documentation in the SI, section 9. If the sourcing season was unknown, an annual average amount²² of heating oil (fossil fuel) per crop was used for one growing period. All productions in Switzerland and further north were modeled as heated and nonheated to approximate a winter and a summer production respectively. All productions south of Switzerland were assumed to be nonheated.

Irrigation. Irrigation is needed in regions where rainfall is less than the amount of water required to grow a specific crop, where rainfall is seasonally unevenly distributed or if crops are cultivated in greenhouses. The amount of water irrigated depends on the culture as well as on soil and different climate parameters like temperature, wind and rainfall. The different amounts of irrigation water for all the crops grown in Switzerland are available from elsewhere.²² Short-term crops (like lettuce and radish) and open field crops use 400–800 m³/ha/growing cycle, long-term greenhouse crops use 3000–6000 m³/ha/growing cycle.²² The irrigation inventory for imported crops was calculated according to Pfister et al.²⁷ As only the country of origin was known, a production weighted average amount was used, taking into account the geographical distribution of each crop within a country.

Transportation. Domestic production covers 40% and 49% of the fruit and vegetable consumption respectively,²⁸ whereas the rest is imported. Imported products have to be transported to and distributed within Switzerland. Distribution is also required for domestic production. The most important production sites in a country were identified for each product

and the most evident transportation routes and means were chosen according to the scheme in Table S4 (SI, section 11). It was assumed that trucks from industrial countries are EURO 4 or 5 standard with cargo weight >32 t, except for distribution in Switzerland, which was modeled with a specific fleet average truck of >28 t. Truck-transportation in emerging economies was simulated with an EURO 3 standard for cargo weight >32 t. By sea route the products are transported by freight ship and in the air by an intercontinental freight aircraft. The corresponding ecoinvent processes were employed and distances were measured with online tools (SI, section 11).

Cooling during Transportation. Crops need to be cooled in order to avoid decay before arriving at the point of sale and to elongate the storage life. Transportation was assumed to take place in fully loaded ISO-containers with independent cooling aggregates. According to Wild²⁹ the average power consumption of a container is 3.6 kW/h·TEU. One TEU (= twenty-foot equivalent unit) is the size of a little standardized container with an average load of 10 t.³⁰ Furthermore, the transportation time (SI, section 12) was needed to model the consumed cooling energy with the ecoinvent data set “diesel electric generating set”.

Washing Water. Several crops (asparagus, bananas, carrots, celery root, cucumbers, iceberg lettuce, lettuce, radish, spinach, and zucchini) need to be cleaned after harvesting. It was assumed that 0.4 L of tap water is used per kg of crop, except for bananas which use 4.4 L per kg.³¹

Electricity Use for Storage. Agricultural goods are stored in refrigerated units. Energy consumption depends on storage time, outside temperature, ideal storage temperature (crop specific) ranging from −2 to 13 °C^{32–37} and packing density, which is generally assumed to be 300 kg/m³.³⁰ Information on energy consumption was extrapolated from elsewhere.¹³

Fertilizer Emissions. Nitrate and phosphorus-emissions into different compartments were modeled generically, because no site-specific values of the productions sites (slope, soil, machine type, weather etc.) were available. On average, 6% of ammonium nitrate fertilizer is emitted into the air as ammonia (NH₃), 1.7% as nitric oxide (NO) and the same amount as nitrous oxide (N₂O) into the air as well, whereas 35% is estimated to be leached as nitrate (NO₃) into the soil.³⁸ Constant values of phosphate emission into groundwater (0.07 kg phosphate/ha/a) and of phosphorus emission into surface water (0.245 kg phosphorus/ha/a) were assumed.³⁹

Other Processes. Assumptions and data about mulch film application and flame treatment are documented in the SI, section 6 and 7.

Life Cycle Impact Assessment. The elaborated LCI data can be coupled with any LCIA method. In this paper, we show selected results for the impact categories climate change⁴⁰ and water stress.⁴¹ Results in terms of a LCIA method using multiple impact categories were calculated with ReCiPe⁴² and are shown in the SI, section 14. Human toxicity impacts due to pesticide use, if applied properly, were shown to be relatively small in relation to “other” impacts like GWP⁴ and were excluded in this study.

Prioritization of Crops. In order to efficiently identify improvement potentials, crops were first ranked according to the impact caused by the total sales volume of a crop ($IS_{c,total}$ in eq 1):

$$IS_{c,total} = \sum_i \sum_j m_{c,i,j} \cdot is_{c,i,j} \quad (1)$$

where $is_{c,ij}$ is the specific impact score per kg of crop c from origin i and produced with mode of production/transportation j , and $m_{c,ij}$ is the respective mass of crop c sold by the retailer.

In addition to the total impact, the sales-amount weighted average impact per kg of product and the variation in specific impact across different origins, production techniques and mode of transportation were also taken into consideration. Priority crops for an in-depth investigation were selected by quantifying the maximal (not necessarily realistic) improvement potential per crop according to eq 2:

$$I_c = \frac{m_{c,\text{total}}(is_{c,\text{average}} - is_{c,\text{min}})}{IS_{c,\text{total}}} \quad (2)$$

where I_c is the maximal improvement potential for crop c (in % of total current impact), $m_{c,\text{total}}$ is the total mass of crop c sold, $is_{c,\text{average}}$ is the sales-amount weighted impact score per kg of crop c and $is_{c,\text{min}}$ the minimal specific impact for crop c found in the considered origins and mode of production/transportation. Those crops for which the sum of the improvement potentials was larger than one-third of the current CO_2 -footprint⁴³ were selected for in-depth analysis.

RESULTS

Carbon Footprint. Figure 2 shows the CO_2 -footprint of fruit and vegetable sales, calculated according to eq 1 (Figure 2a) and the specific CO_2 -footprint with its variation (Figure 2b).

Asparagus, lettuce and cucumbers were selected for in depth investigation, to derive high-leverage recommendations for a reduction in environmental impact. Switching to the respective production alternative with minimal impact for these three crops would achieve a reduction of more than one-third of the current overall CO_2 -footprint caused by the sale of all crops considered (Table 1). Tomato also exhibits a relatively high improvement potential.

Other crops like bananas, pears, apples, citrus fruits, and potatoes also cause a relatively large total CO_2 -footprint because of large amounts sold, but due to their small specific impact the potential for improvement is limited.

Asparagus was clearly the most important crop to be analyzed according to the ranking scheme applied. Figure 3 shows that the main load of the GWP originates from air transport from Mexico and Peru. The carbon footprint of different origins and transportation options differs by a factor of 16–19, respectively, from the lowest (produced locally in Switzerland) to the highest (imported by airplane from Mexico (green asparagus) and Peru (white asparagus)). Therefore, a recommendation to reduce air transport and to encourage seasonal production from near regions was derived.

For the remaining crops, classified as “high priority to reduce the carbon footprint”, the main driver of impact was greenhouse heating with fossil fuels during production out of season. For example, a comparison between Swiss cucumber production from unheated and heated greenhouses shows a GWP-difference by a factor of more than 10 (Figure 4). A large difference between heated and nonheated production can also be observed for eggplants (factor of 6), tomatoes and peppers (both factor of 4) and lettuce (factor of 10). Emissions including those from fossil fuel-heating are not evenly distributed over the whole season. The results of the GWP combined with the seasonal heating energy model are shown for a Swiss lettuce production in Figure 4.

Energy demand for cool storage induces less GWP than import by ship from southern countries. For example comparing kiwis imported from Italy and New Zealand, import from Italy is always less CO_2 -eq. intensive, even when considering 36% higher yields, which have been reported for New Zealand.⁴⁴

Different scenarios of the total GWP of the fruits and vegetables assessed reveal a reduction potential of 42% changing from the scenario with air-freighted oversea-asparagus and vegetables produced in heated greenhouses in northern Europe to a supply without air transport and fossil fuel heated greenhouse productions. Without air transport, asparagus alone bears a GWP-reduction potential of 20%. A similar reduction (22%) can potentially be achieved by avoiding vegetables from heated greenhouses and sourcing them from Southern countries during winter and spring, or, even better, from heated greenhouses with waste heat from other industrial processes.

Impacts from Water Consumption. In Figure 5b, the water consumed during the production of selected fruits of different origins is weighted by the water stress index (WSI).⁴¹ Differences in the environmental impact are mostly caused by water scarcity of a specific region and the ratio of irrigated water consumed to the yield. The impact is clearly visible for the asparagus and avocado production (figure 5b), whereas for the other fruits and vegetables it is not. In some cases, a “good water performance” can be in contradiction to a “good GWP performance”, as in the case of citrus fruits from Israel (SI, section 15). In other cases, both indicators are in accordance, such as in the case of seasonal production of fruits and vegetables from Switzerland, which have a low impact with respect to both indicators.

Implemented Measures by the Commissioner of This Study. Several measures have been implemented to reduce the large impact due to air transport. Products transported by air freight are declared with a label “by air” and the emissions are fully compensated through offsetting schemes. Through efficient logistics and improved storage techniques the amount of white asparagus transported from overseas by ship was increased from 50–90% from 2007 to 2009. However, green asparagus is still not transported by ship from overseas due to substantial losses. To lower the impact of the green asparagus imported by air-freight the retailer decided not to sell this product at discount prices anymore since spring 2009. With this measure it was possible to reduce the emissions from air-transported asparagus by 75% from 2008 to 2009. In addition, a new production site in Taroudant, Morocco is being established to avoid air transport dependency.⁸ Furthermore, the results of the study were communicated to the purchasing staff (in the forms of a report, a leaflet and a calculation tool) to enable an environmentally informed supply chain management for all products.

DISCUSSION

Recommendations for Decision Making. Airplane transport dominated the carbon footprint of fruits and vegetables, that is, asparagus and papaya. A decision recommendation for consumers could be, for instance, that seasonal consumption of local foods is to be preferred over out-of-season fruits and vegetables that are imported by plane. For retailers it is recommended to avoid long-distance transports or to prefer transport by ship whenever possible. These results are in accordance with the studies of Jungbluth et al.⁴⁵ or Sim et al.,⁴⁶

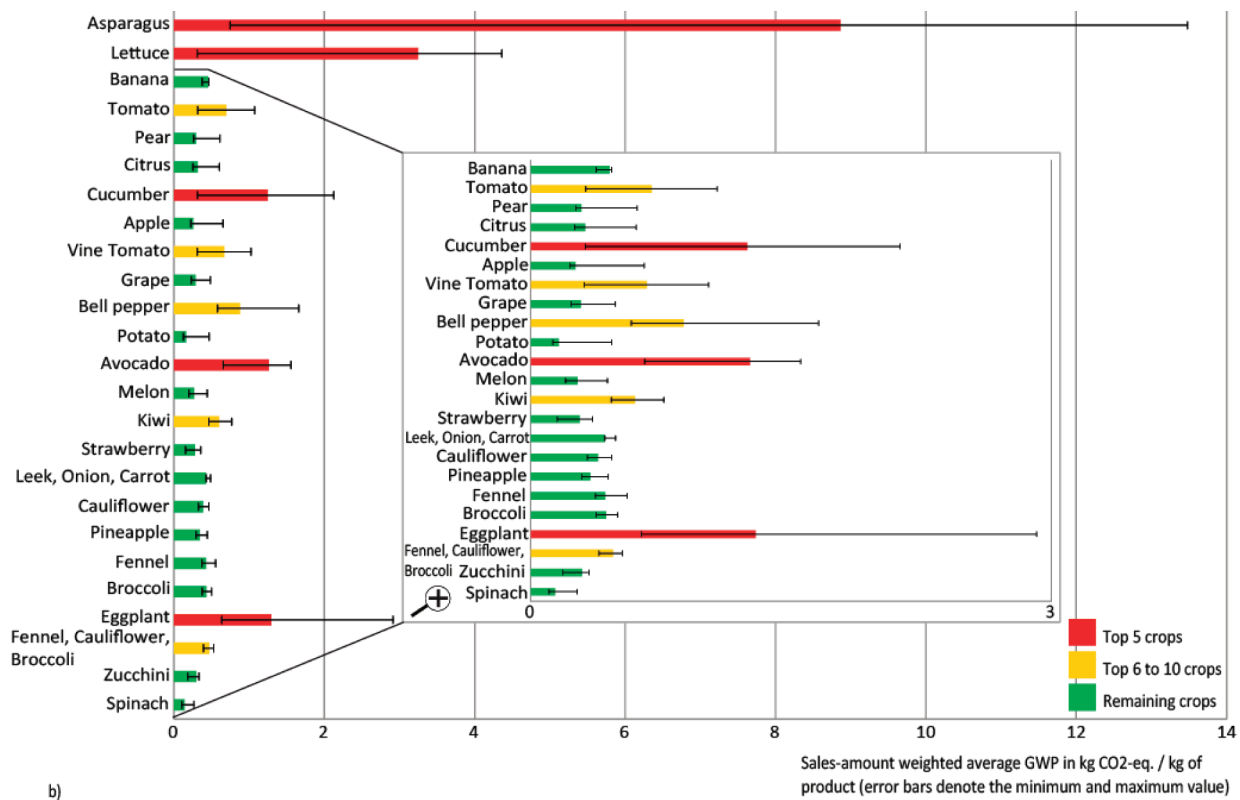
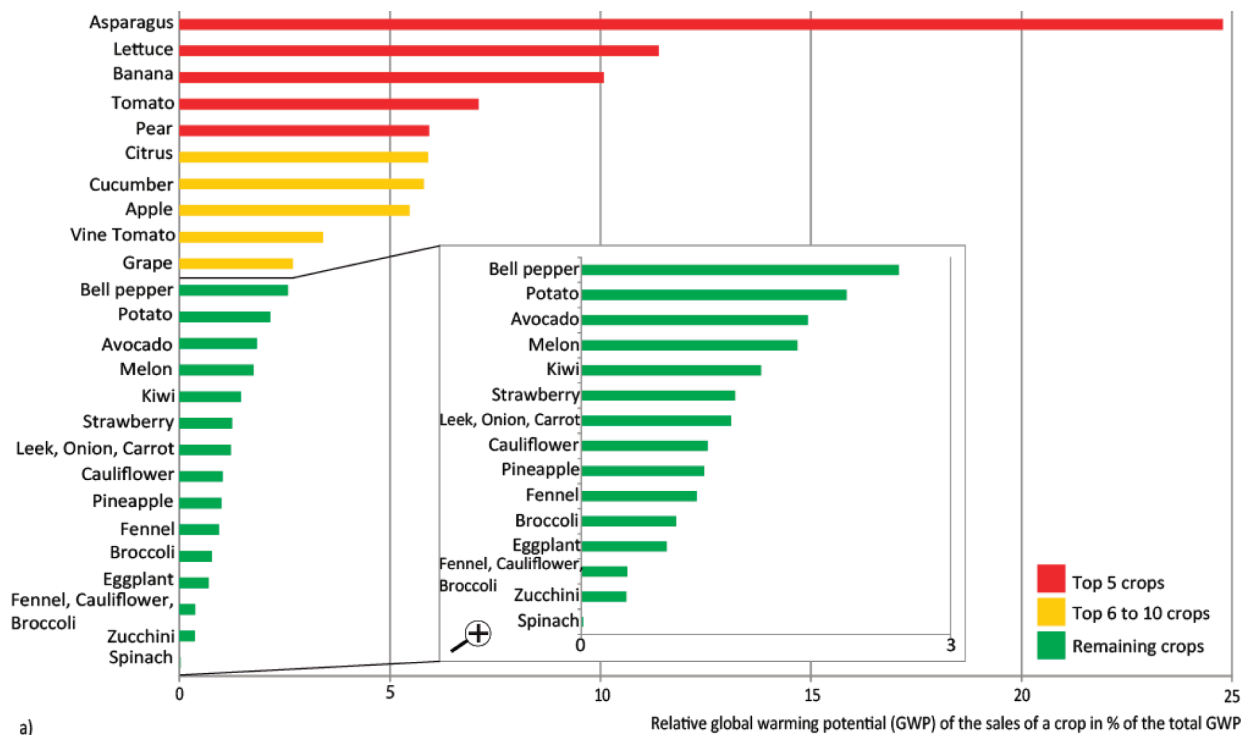


Figure 2. Relative global warming potential (GWP) in % of the total GWP generated by all considered fruits and vegetables sold in 2007 (ordered from top to bottom, 2a) and sales-amount weighted impact per kg of product (2b). The error bars denote the minimum and maximum specific impact over all options assessed (varying origin, means of transportation, production modes, etc.).

but differ from Weber et al.,¹⁹ who conclude that foodmiles in the U.S. are, on the whole, less relevant than agricultural production.

Another general result is that greenhouse heating may be a key process for vegetables that are grown out of season in

colder climates. In many cases, heating greenhouses with fossil fuels was more important than ground transport, even if distances were long (e.g., South Spain to Switzerland). Thus, during winter and spring it is often better to purchase vegetables that are grown in greenhouses from Southern countries,

Table 1. Theoretical Improvement Potential in % of Current Overall CO₂ footprint (Only Crops >1% Displayed), Calculated According to eq 2

	theoretical improvement potential (%)
asparagus	22.7
lettuce	10.3
cucumber	4.3
tomato	3.9
vine tomato	1.8
banana	1.7
citrus	1.2

where no heating is needed, while during summer or fall, local production is often better than imports. However, there is often a trade-off between the relatively low carbon footprint of winter and spring production in Southern countries and the water stress induced in these countries, a situation that needs to be carefully assessed case by case. The use of heating systems with nonfossil energy and particularly waste heat could be a solution which may reduce both carbon footprint and water stress impacts. Some greenhouses functioning with waste heat are already in operation, for example, the greenhouse attached to a municipal solid waste incineration in Hinwil,⁴⁷ and the tropical centers in Frutigen and Wollhusen, Switzerland,⁴⁸ which are heated with geothermal heat (warm water effluent from a tunnel) and waste heat from a gas concentration unit respectively. The decision recommendation for food producers would thus be to search for such alternative heat energy sources or to avoid heating as much as possible. The latter is already standard practice for organic producers in Switzerland, as heating is only permitted to avoid harvest losses from freezing temperatures according to the standards of Bio Suisse.⁴⁹

Retailers in northern countries can lower the CO₂-eq. emissions by sourcing their greenhouse-grown products locally during the season. In winter and spring they should look for imports from warmer locations, provided that there are no adverse effects such as water stress (and further impacts not investigated here). Retailers are suggested to use results from LCA studies, to decide where to source each fruit and vegetable from, and which aspects to improve in collaboration with the producers in each case. They could also label best-practice products, although the communication of LCA-results to consumers is a challenging task and consumer organizations already warn against too much and too complex information on products.^{50,51} Finally, consumers should buy seasonal products or local products that can be stored over the season as much as possible to avoid both long-distance and air transport, as well as greenhouse heating. Moreover, it is desirable that crops with low specific impact are consumed in large amounts, as is already the case for pear, grape, potato, melon, carrot, etc. To enable such decisions, policy makers should ensure that retailers label the origin, transportation, and mode of production of their products.

Storage energy is in some cases significant, and efficient cooling technologies are fairly important. Nevertheless, local production combined with long storage tends to perform better than long-distance imports from countries like New Zealand, which is for certain crops, such as kiwi and apple, a relevant country for imports into Switzerland. Our results are in accordance with Blanke et al.,⁵² but in contradiction with

Milà i Canals,⁵³ who considered 5–40% loss for apples which are stored for 4–10 months. The latter assumption is justified for apples consumed in European spring.

In many purchasing decisions, retailers or consumers can generate significant savings in environmental impacts by following simple guidelines as outlined above. Although the study has been made for a Swiss retailer, the LCI data are adaptable to assortments of other retailers worldwide.

Data Uncertainty. Some key pieces of information about the supply chain like crop, origin, transportation mode, and sales numbers were provided by the retailer. The inventory data are based on this information and use generic data for the production processes, for example, Swiss averages from the horticultural association, which produces according to GAP. However, it should be noted that variability is large between regions and even between farms.^{54,55} For example, eutrophying emissions are a function of many parameters including climatic factors. Thus, our average data is rather uncertain and may need to be revised particularly for countries without GAP-tradition in the field of fertilization, yield and machinery use and in case the data is applied to retailers which do not make sure that GAP is followed by all suppliers. One possibility of how to do that is proposed by Roches et al.⁵⁶ Similar adaptations may be used for a comparison between farms.

The storage lives of the analyzed products vary from 10 days to half a year, something which has, among other factors, an influence on the amount of food losses. Food losses may be significant⁵⁷ and should be assessed, although we were not able to collect representative data within this study. Data on food losses are specific for each retailer, supply chain and crop. Thus, such data should be added to the inventory data when performing LCA studies.

Implementation Illustrated for the Case of a Specific Retailer. In the particular case of the commissioner of this study, it was decided that the highest leverage decisions can be taken on the levels of purchasing decisions of the retailers and communication to producers. The rationale was that only sustainable products should be offered (also for social standards which are not discussed in this paper), so that the consumers can buy any product without violating minimum standards and the vast majority of customers is covered. Additionally, consumer information such as origin and mode of production of all fruits and vegetables are provided so that environmentally educated consumers have the chance to choose the environmentally friendliest product among those offered.

The results of the implemented measures shows that the reduction potential identified by a LCA-analysis and implemented into daily business can lower the overall impact without substantially compromising the company economically. It also demonstrates the opportunities of retailers for reducing environmental impacts of food consumption.

OUTLOOK

Food products are known to have significant environmental impacts other than climate change and water use impacts. Those other potential impacts should be covered in a LCA complementing the carbon and water evaluation to avoid problem shifting. Further environmental effects of concern include impacts from land use, eutrophication and toxic effects. While for some of these impacts (e.g., ecotoxicity and eutrophication) standard assessment methods exist, methodological developments are needed for others (e.g., soil

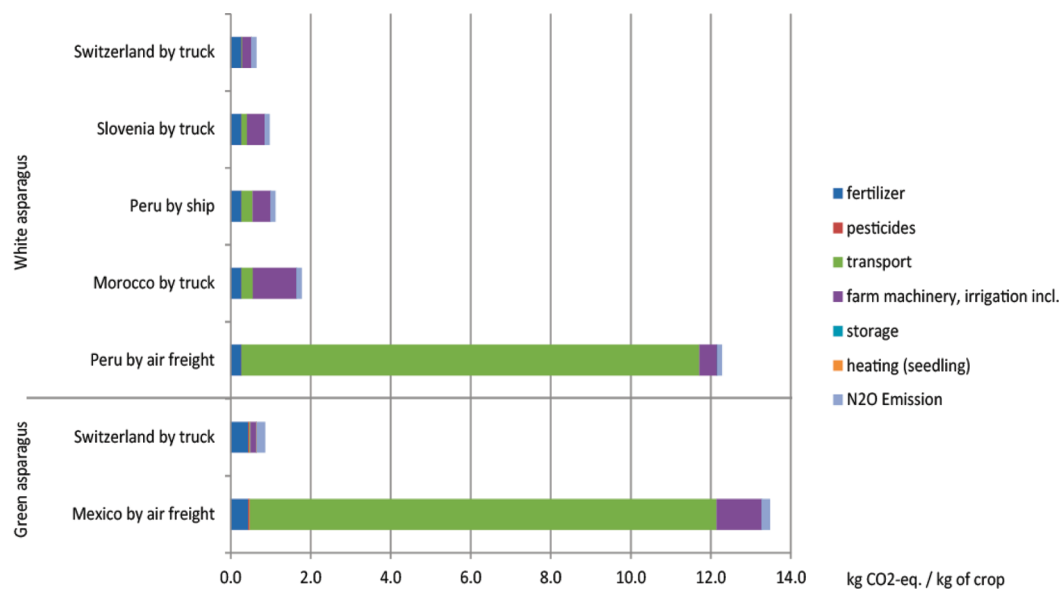


Figure 3. GWP of green and white asparagus imported to Switzerland from different countries of origin.

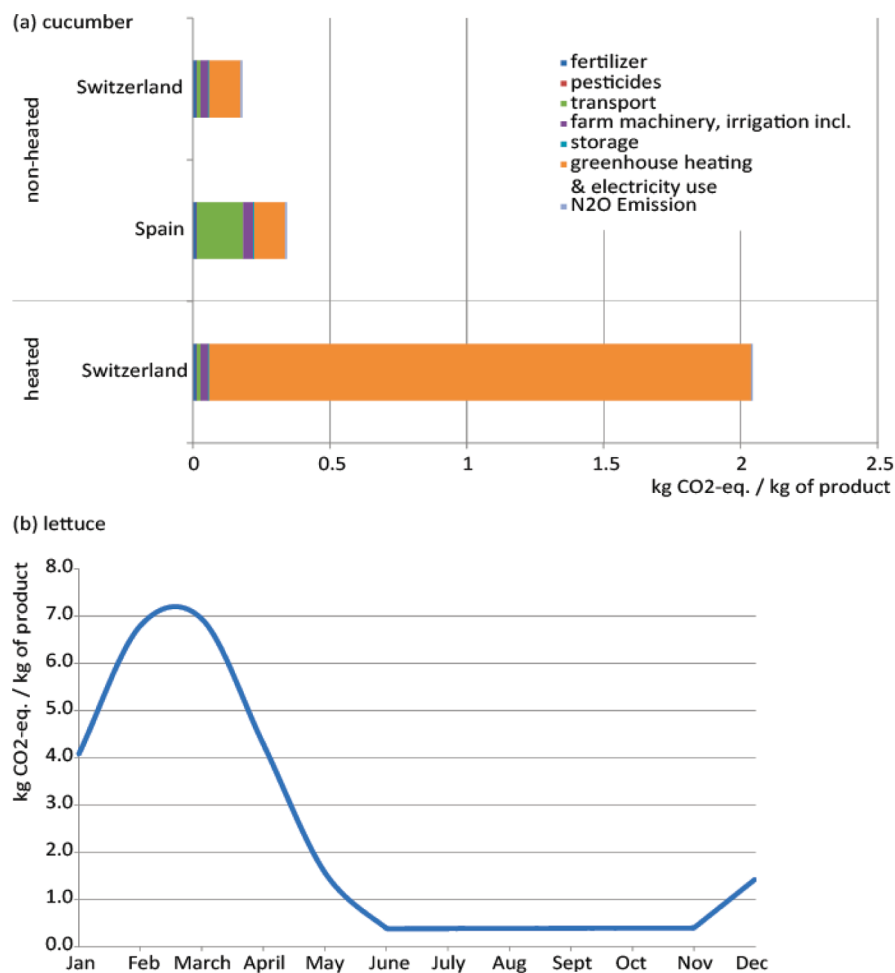


Figure 4. GWP of cucumbers grown either unheated or in (with an annual average amount of heating oil) fossil fuel heated greenhouses (a). GWP of lettuce at harvesting time produced in a greenhouse for a year-round production (b).

fertility, erosion, salinization, and biodiversity impacts⁵⁸). A complete LCIA including these impact categories is also needed for a fair comparison between organic and intensive production systems.

Furthermore, the assessment could be expanded to an analysis from cradle to grave, including the use phase (transport from the store to where it is consumed, preparation like e.g. cooking, etc.) and especially the food losses over the whole chain.

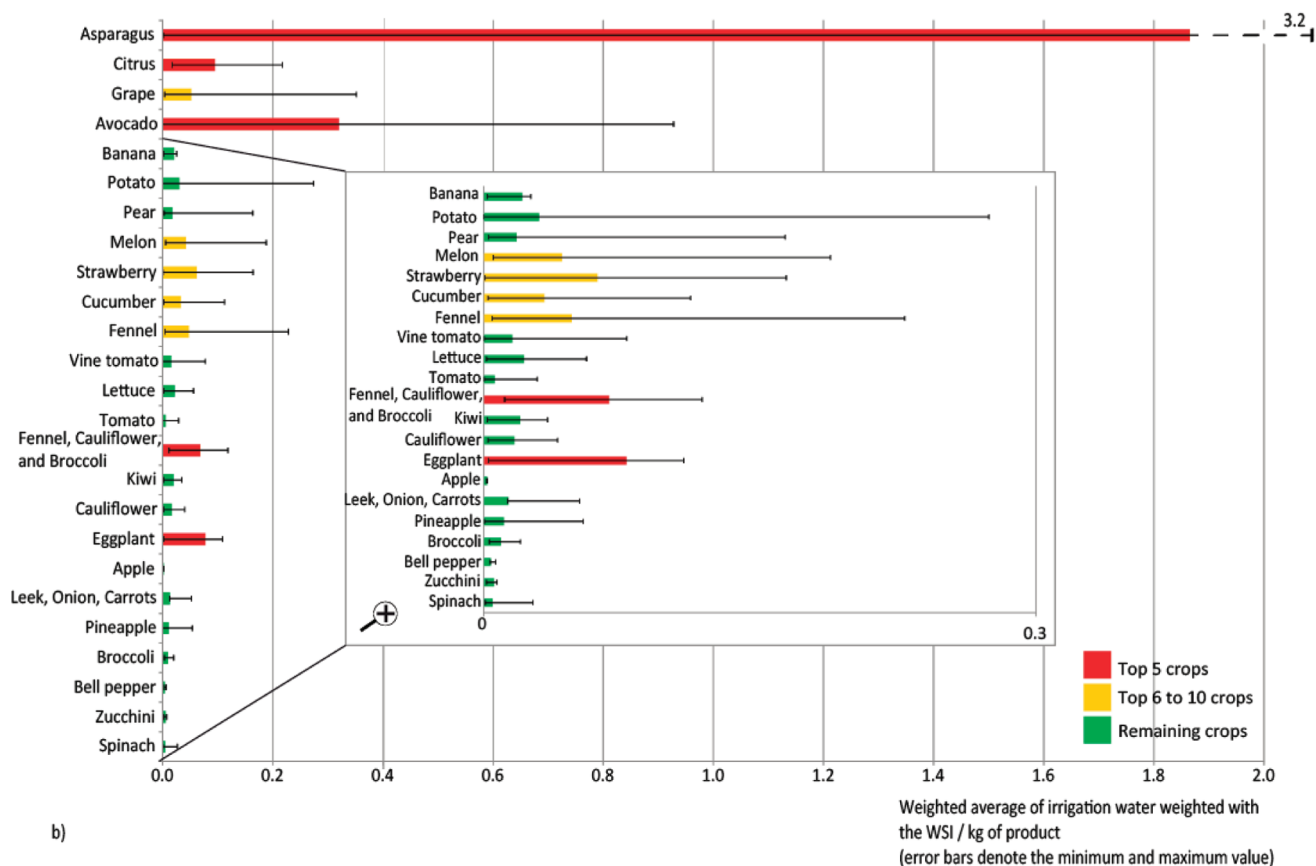
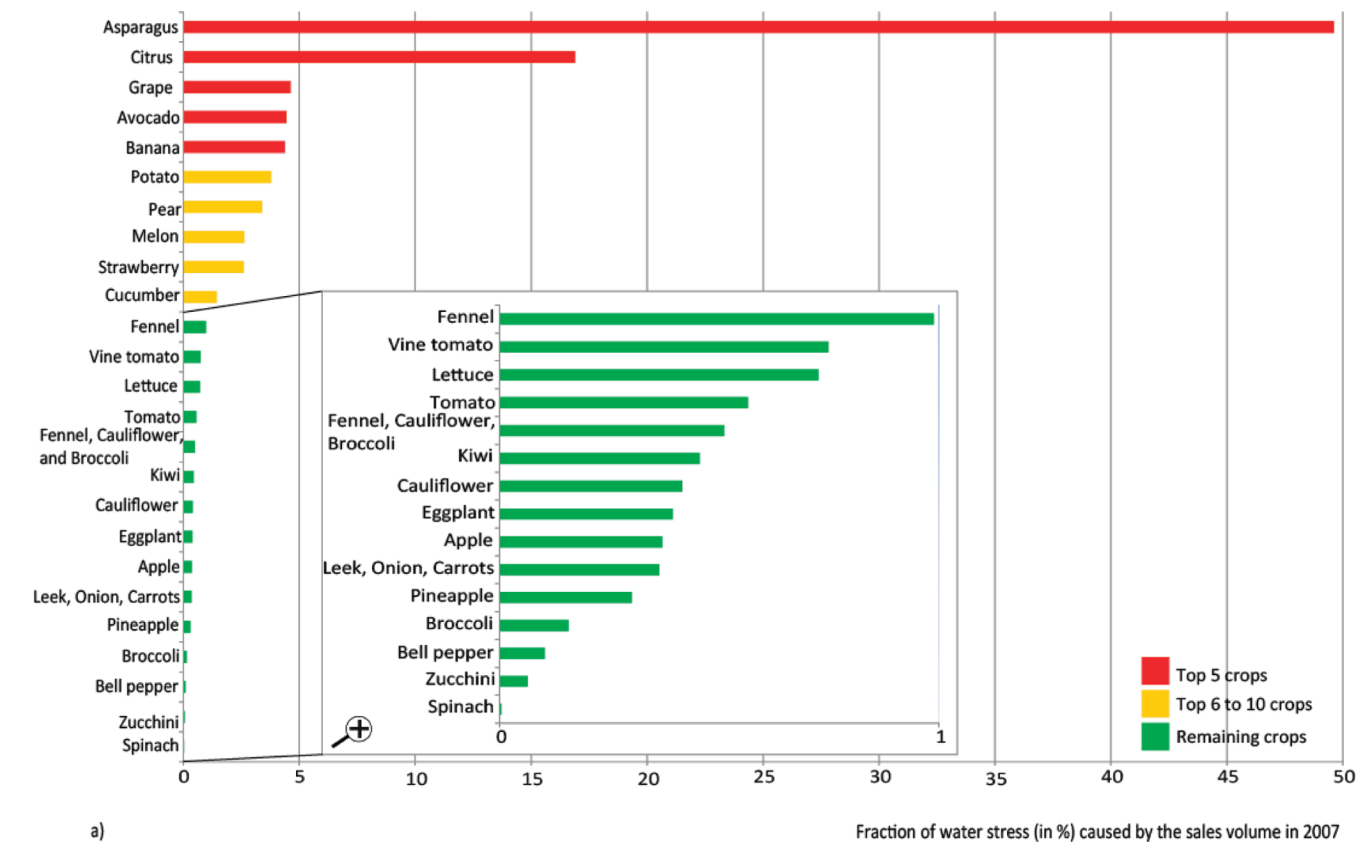


Figure 5. Fraction of water stress (in % and ordered from top to bottom) caused by the sales volume in 2007 normalized by the sum of water stress of all crops (5a) and sales-amount weighted water stress (irrigation water (m³)·WSI) per kg of (5b).

■ ASSOCIATED CONTENT

■ Supporting Information

Additional material as noted in the text. This information is available free of charge via the Internet at <http://pubs.acs.org>

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